

Photon position eigenvectors lead to complete photon wave mechanics

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ABSTRACT

We have recently constructed a photon position operator with commuting components. This was long thought to be impossible, but our position eigenvectors have a vortex structure like twisted light. Thus they are not spherically symmetric and the position operator does not transform as a vector, so that previous non-existence arguments do not apply. We find two classes of position eigenvectors and obtain photon wave functions by projection onto the bases of position eigenkets that they define, following the usual rules of quantum mechanics. The hermitian position operator, \hat{r}_0 , leads to a Landau-Peierls wave function, while field-like eigenvectors of the nonhermitian position operator and its adjoint lead to a biorthonormal basis. These two bases are equivalent in the sense that they are related by a similarity transformation. The eigenvectors of the nonhermitian operators $\hat{r} \pm 1/2$ lead to a field-potential wave function pair. These field-like positive frequency wave functions satisfy Maxwell's equations, and thus justify the supposition that MEs describe single photon wave mechanics. The expectation value of the number operator is photon density with undetected photons integrated over, consistent with Feynman's conclusion that the density of non-interacting particles can be interpreted as probability density.

1. INTRODUCTION

It has been claimed since the early days of quantum mechanics that there is no position operator for the photon, and thus that a real space wave function cannot be obtained in the usual way, by projection of the state vector onto a basis of position eigenvectors. Quite recently we have succeeded in constructing photon position operators with commuting components whose transverse eigenvectors form bases of localized states.¹⁻³ These Hermitian and pseudo-Hermitian bases can be used to derive photon wave functions in the usual way, leading to a real space description of the photon that is compatible with all of the usual rules of quantum mechanics.⁴ It is this new photon wave mechanics that will be discussed here.

2. $M > 0$ WAVE MECHANICS

In the standard formulation of quantum mechanics an observable is described by an operator, \hat{o} , whose eigenvalues, o_n , are the possible results of a measurement of that observable. If the state vector is expanded in its complete set of eigenvectors, $\{|\phi_n\rangle\}$, the squares of the coefficients in this expansion are the probabilities for the corresponding eigenvalue to be measured, that is

$$\begin{aligned}\hat{o}|\psi_n\rangle &= o_n |\psi_n\rangle, \\ |\Psi\rangle &= \sum_n c_n |\psi_n\rangle, \\ |c_n|^2 &= \text{probability to get } o_n.\end{aligned}$$

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If the observable is position, the spectrum of eigenvalues becomes continuous so that

$$\begin{aligned}\hat{\mathbf{r}}|\phi_{\mathbf{r}'}\rangle &= \mathbf{r}'|\phi_{\mathbf{r}'}\rangle, \\ |\Psi\rangle &= \int d^3r' c(\mathbf{r}')|\phi_{\mathbf{r}'}\rangle, \\ |c_{\mathbf{r}'}|^2 &= \text{probability density to find the particle at } \mathbf{r}'.\end{aligned}\tag{1}$$

In real space the position operator of a massive particle such as an electron is $\hat{\mathbf{r}} = \mathbf{r}$ and the position eigenvectors are the 3-dimensional Dirac δ -functions,

$$\psi_{\mathbf{r}'}(\mathbf{r}) = \delta^3(\mathbf{r} - \mathbf{r}'),$$

localized at \mathbf{r}' . The \mathbf{k} -space description of these localized states is their inverse Fourier transform,

$$\begin{aligned}\psi_{\mathbf{r}'}(\mathbf{k}) &= \int d^3r \delta^3(\mathbf{r} - \mathbf{r}') \frac{\exp(-i\mathbf{k} \cdot \mathbf{r})}{\sqrt{V}} \\ &= \frac{\exp(-i\mathbf{k} \cdot \mathbf{r}')}{\sqrt{V}},\end{aligned}$$

while the position operator becomes

$$\hat{\mathbf{r}} = i\nabla.\tag{2}$$

Here ∇ is the \mathbf{k} -space gradient operator whose j^{th} Cartesian component is $\nabla_j = \partial/\partial k_j$.

3. GLAUBER WAVE FUNCTION

In spite of the widely held belief that there is no photon position operator and hence no first quantized description of the photon, many quantum optics researchers consider a photon wave function to be highly desirable. This was the subject of a number of papers at the 2005 SPIE conference on The Photon and in a special issue of Optics and Photonics News.⁵ A wave function can be introduced through Glauber photodetection theory.⁶ The Glauber probability per unit time that a photon will be absorbed by a negligibly small detector at point \mathbf{r} and time t for an electromagnetic field in state $|\Psi\rangle$ is

$$\frac{dn_G}{dt} \propto \left\langle \Psi \left| \hat{\mathbf{E}}^{(-)}(\mathbf{r}, t) \cdot \hat{\mathbf{E}}^{(+)}(\mathbf{r}, t) \right| \Psi \right\rangle.\tag{3}$$

The 1-photon wave function is then defined as the probability amplitude^{7,8}

$$\Psi^{(1/2)}(\mathbf{r}, t) = \left\langle 0 \left| \hat{\mathbf{E}}^{(+)}(\mathbf{r}, t) \right| \Psi \right\rangle.\tag{4}$$

The superscript 1/2 used here denotes the quantum electrodynamics (QED) $(\omega_k)^{1/2}$ dependence of the field operator

$$\hat{\mathbf{E}}^{(+)}(\mathbf{r}, t) \equiv \sum_{\mathbf{k}} \mathcal{C}(\omega_k)^{1/2} \mathbf{e}_{\mathbf{k}, \sigma}^{(\chi)} a_{\mathbf{k}, \sigma} \frac{e^{i\mathbf{k} \cdot \mathbf{r} - i\omega_k t}}{\sqrt{V}}\tag{5}$$

where $\omega_k = kc$ in free space. This is consistent with the QED based interpretation that a mode with frequency ω_k has energy $\hbar\omega_k$. Since the square of the field must give energy density, terms must be weighted by the factor $\sqrt{\omega_k}$. The operator $a_{\mathbf{k}, \sigma}$ annihilates a photon with wave vector \mathbf{k} and polarization σ and $\mathcal{C} \equiv \sqrt{\hbar/2\epsilon_0 V}$. This wave function is useful, but its square is not a probability density, and it cannot be incorporated into the usual quantum mechanical framework.

There are a number of other candidates for photon wave function in the literature.¹¹ In particular, the Landau-Peierls (LP) wave function,⁹ $\Psi^{(0)}(\mathbf{r}, t)$, omits the $\sqrt{\omega_k}$ dependence. Its absolute value squared, $n^{(0)}(\mathbf{r}, t) = |\Psi^{(0)}(\mathbf{r}, t)|^2$, is then a local and positive definite photon number density. This wave function has the disadvantage that its relationship to current is nonlocal. Equations of motion and probability density based on $\hat{\Psi}^{(0)}$ was investigated by Mandel and Cook.¹⁰ To allow for both LP and field-like wave function we will consider a frequency dependence of the form $(\omega_k)^\alpha$ here.

4. SPIN AND HELICITY

The photon helicity is the component of spin in the direction of propagation, that is in the \mathbf{k} -direction. We will work in \mathbf{k} -space, which is equivalent to momentum space. The localized basis states that we will use here have definite helicity, but they do not have definite spin or orbital angular momentum (AM) along any fixed direction in space. Since it is important to understand these distinctions, we will first consider the z -components of orbital AM, spin, and helicity in units of \hbar ,

$$\hat{L}_z = i \frac{\partial}{\partial \phi}, \quad (6)$$

$$S_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (7)$$

$$S_{\mathbf{k}} = \hat{\mathbf{k}} \cdot \mathbf{S}. \quad (8)$$

The Cartesian components of the spin 1 operator are the 3×3 matrices $(S_i)_{jk} = -i\epsilon_{ijk}$, with its z -component being given explicitly in (7). The eigenvectors of \hat{L}_z are $\exp(il_z\phi)/\sqrt{2\pi}$ with eigenvalue $\hbar l_z$, while those of \hat{S}_z are $\mathbf{e}_{s_z} = (\hat{\mathbf{x}} + is_z\hat{\mathbf{y}})/\sqrt{2}$ with eigenvalue $s_z = \pm 1$ and $\mathbf{e}_0 = \hat{\mathbf{z}}$ with eigenvalue $s_z = 0$. The unitary transformation

$$D = \exp(-iS_z\phi) \exp(-iS_y\theta) \quad (9)$$

rotates the Cartesian unit vectors, $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}\}$, to the spherical polar unit vectors $\{\hat{\theta}, \hat{\phi}, \hat{\mathbf{k}}\}$. It transforms S_z to the helicity operator $S_{\mathbf{k}} = DS_zD^{-1}$ and the S_z eigenvectors, $(\hat{\mathbf{x}} + is_z\hat{\mathbf{y}})/\sqrt{2}$, to $\mathbf{e}_{\mathbf{k},\sigma}^{(0)} = D\mathbf{e}_{s_z}$ where

$$\mathbf{e}_{\mathbf{k},\sigma}^{(0)} = (\hat{\theta} + i\sigma\hat{\phi})/\sqrt{2}. \quad (10)$$

This preserves eigenvalues so that unit vectors $\mathbf{e}_{\mathbf{k},\sigma}^{(0)}$ have definite helicity $\sigma = \pm 1$, while $\mathbf{e}_{\mathbf{k},0}^{(0)} = \hat{\mathbf{k}}$ has eigenvalue 0. The unit vectors are no longer fixed, since $\hat{\theta}$ and $\hat{\phi}$ depend on $\hat{\mathbf{k}}$.

5. POSITION OPERATOR

In the absence of free charge the displacement and magnetic induction vectors satisfy $\nabla \cdot \mathbf{D} = 0$ and $\nabla \cdot \mathbf{B} = 0$, that is these fields are transverse. In the Coulomb gauge the vector potential is also transverse. In \mathbf{k} -space space this condition reduces to $\mathbf{k} \cdot \mathbf{D} = 0$ and $\mathbf{k} \cdot \mathbf{B} = 0$, and the spherical polar unit vectors $\hat{\theta}$ and $\hat{\phi}$ provide a basis for the description of these transverse vectors. We will use the equivalent $\mathbf{e}_{\mathbf{k},\sigma}^{(0)}$ basis here, since eigenvectors of the helicity operator provide us with a complete set of commuting observables (CSCO), namely helicity and the components of the position operator. Transverse wave functions of the form¹

$$\psi_{\mathbf{r},\sigma,j}^{(\alpha)}(\mathbf{k}) = (\omega_k)^\alpha e_{\mathbf{k},\sigma,j}^{(\chi)} \exp(-i\mathbf{k} \cdot \mathbf{r}) / \sqrt{V} \quad (11)$$

describe a photon with helicity σ located at position \mathbf{r} . Here subscripts denote eigenvalues and Cartesian components of the vectors ψ and \mathbf{e} , and Cartesian components are used where it is necessary to avoid confusing vector notation. The parameter α describes electric and/or magnetic fields if $\alpha = 1/2$, the vector potential if $\alpha = -1/2$, or LP wave functions if $\alpha = 0$. Periodic boundary conditions in a finite volume are used here to simplify the notation, and the limit as $V \rightarrow \infty$ can be taken to calculate derivatives and perform sums.

If the wave function (11) is a position eigenvector it should satisfy the eigenvector equation (1), that is

$$\hat{\mathbf{r}}^{(\alpha)} \psi_{\mathbf{r},\sigma,j}^{(\alpha)}(\mathbf{k}) = \mathbf{r} \psi_{\mathbf{r},\sigma,j}^{(\alpha)}(\mathbf{k}) \quad (12)$$

where $\hat{\mathbf{r}}^{(\alpha)}$ is the \mathbf{k} -space representation of the position operator and its eigenvalues, \mathbf{r} , can be interpreted as photon position. The operator that satisfies (12) is¹

$$\hat{\mathbf{r}}^{(\alpha)} = iI\nabla - iI\alpha\hat{\mathbf{k}}/k + \hat{\mathbf{k}} \times \mathbf{S}/k + S_{\mathbf{k}}\hat{\phi} \cot \theta/k \quad (13)$$

where I is a 3×3 unit matrix. Eq. (13) looks cumbersome, but it has a simple interpretation. The position information is contained in the phase factor, $\exp(-i\mathbf{k} \cdot \mathbf{r})$. The position operator (13) can be rewritten as²

$$\hat{\mathbf{r}}^{(\alpha)} = D \left[(\omega_k)^\alpha i\nabla (\omega_k)^{-\alpha} \right] D^{-1}.$$

The interpretation of this is that, starting from a wave vector parallel to $\hat{\mathbf{z}}$ and transverse unit vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$, D rotates \mathbf{k} from the z -axis to an orientation described by the angles θ and ϕ , while at the same time rotating the transverse vectors to $\hat{\theta}$ and $\hat{\phi}$ to give (10). The factor $(\omega_k)^{-\alpha}$ removes the $(\omega_k)^\alpha$ dependence in (11). For example, when $\hat{\mathbf{r}}^{(1/2)}$ acts on a transverse field parallel to $\hat{\phi}$, D^{-1} rotates it to $\hat{\mathbf{y}}$ and divides it by $\sqrt{\omega_k}$, leaving only the phase factor which it operates on it with the usual \mathbf{k} -space position operator, $i\nabla$ (11). The process is then reversed by multiplying by $\sqrt{\omega_k}$ and using D to rotate the eigenvector back to its original transverse orientation. This allows $\hat{\mathbf{r}}^{(1/2)}$ to extract the position of the photon from $\exp(-i\mathbf{k} \cdot \mathbf{r})$ while ignoring other factors.

The position operator can be generalized to allow for rotation about \mathbf{k} through the Euler angle $\chi(\theta, \phi)$ to give the most general transverse basis,²

$$\mathbf{e}_{\mathbf{k},\sigma}^{(\chi)} = e^{-i\sigma\chi} \mathbf{e}_{\mathbf{k},\sigma}^{(0)}. \quad (14)$$

The quantum numbers $\{\mathbf{r}, \sigma\}$ index the basis states of the CSCO for a given $\chi(\theta, \phi)$. The z -axis can be selected for convenience and the choice $\chi = -m\phi$ then gives³

$$\begin{aligned} \mathbf{e}_{\mathbf{k},\sigma}^{(-m\phi)} &= \frac{\hat{\mathbf{x}} - i\hat{\mathbf{y}}}{2\sqrt{2}} (\cos\theta - \sigma) e^{i(m\sigma+1)\phi} - \frac{\hat{\mathbf{z}}}{\sqrt{2}} \sin\theta e^{im\sigma\phi} \\ &\quad + \frac{\hat{\mathbf{x}} + i\hat{\mathbf{y}}}{2\sqrt{2}} (\cos\theta + \sigma) e^{i(m\sigma-1)\phi}. \end{aligned} \quad (15)$$

For example, $\chi = -\phi$ ($m = 1$) rotates $\hat{\theta}$ and $\hat{\phi}$ back to the x and y axes to give unit vectors that approach $(\hat{\mathbf{x}} + i\sigma\hat{\mathbf{y}})/\sqrt{2}$ in the $\theta \rightarrow 0$ paraxial limit that describes the optical beams commonly available in the laboratory.

6. INNER-PRODUCT AND SIMILARITY TRANSFORMATION

The $\alpha = 0$ position operator is Hermitian but, for $\alpha = \pm 1/2$, $\hat{\mathbf{r}}$ can be Hermitian or pseudo-Hermitian depending on the choice of inner-product, as will be argued next. The LP inner-product is

$$\langle \Psi^{(0)} | \tilde{\Psi}^{(0)} \rangle = \sum_{\mathbf{k},j} \Psi_j^{(0)*}(\mathbf{k}) \tilde{\Psi}_j^{(0)}(\mathbf{k}), \quad (16)$$

and it can be verified using integration by parts that $\langle \Psi^{(0)} | \hat{\mathbf{r}}^{(0)} \tilde{\Psi}^{(0)} \rangle = \langle \hat{\mathbf{r}}^{(0)} \Psi^{(0)} | \tilde{\Psi}^{(0)} \rangle$, which implies that $\hat{\mathbf{r}}^{(0)}$ is Hermitian. Alternatively, the usual rules for calculating adjoints give

$$\begin{aligned} \hat{\mathbf{r}}^{(0)\dagger} &= \left(iI\nabla + \hat{\mathbf{k}} \times \mathbf{S}/k + S_{\mathbf{k}} \hat{\phi} \cot\theta/k \right)^\dagger \\ &= iI\nabla + \hat{\mathbf{k}} \times \mathbf{S}/k + S_{\mathbf{k}} \hat{\phi} \cot\theta/k = \hat{\mathbf{r}}^{(0)} \end{aligned}$$

which confirms that $\hat{\mathbf{r}}^{(0)}$ is Hermitian. However, application of the same rules to the $\alpha = 1/2$ case gives

$$\begin{aligned} \hat{\mathbf{r}}^{(1/2)\dagger} &= \left(iI\nabla - \frac{1}{2}iI\alpha\hat{\mathbf{k}}/k + \hat{\mathbf{k}} \times \mathbf{S}/k + S_{\mathbf{k}} \hat{\phi} \cot\theta/k \right)^\dagger \\ &= iI\nabla + \frac{1}{2}iI\alpha\hat{\mathbf{k}}/k + \hat{\mathbf{k}} \times \mathbf{S}/k + S_{\mathbf{k}} \hat{\phi} \cot\theta/k \\ &= \hat{\mathbf{r}}^{(-1/2)}. \end{aligned}$$

While a field theory inner-product $\langle \Psi^{(1/2)} | \tilde{\Psi}^{(1/2)} \rangle = \sum_{\mathbf{k}, j} k^{-1} \Psi^{(1/2)*}(\mathbf{k}) \tilde{\Psi}^{(1/2)}(\mathbf{k})$ does make $\hat{\mathbf{r}}^{(1/2)}$ Hermitian, this results in a nonlocal photon number density. An alternative approach is to define the inner-product

$$\langle \Psi^{(1/2)} | \tilde{\Psi}^{(-1/2)} \rangle = \sum_{\mathbf{k}, j} \Psi_j^{(1/2)*}(\mathbf{k}) \tilde{\Psi}_j^{(-1/2)}(\mathbf{k}) \quad (17)$$

involving biorthonormal field-potential pairs. The operator pair $\hat{\mathbf{r}}^{(1/2)}$ and $\hat{\mathbf{r}}^{(-1/2)}$ can then be called pseudo-Hermitian.¹³

The LP and field-potential bases are related by a similarity transformation. In linear algebra, a similarity transformation, ρ , of a matrix O with eigenvectors, f_n , is of the form $O \rightarrow \rho O \rho^{-1}$ and $f_n \rightarrow \rho f_n$. Since $O f_n = \lambda f_n$ implies $(\rho O \rho^{-1})(\rho f_n) = \lambda(\rho f_n)$, this transformation preserves the eigenvalues, λ . If $\rho^{-1} = \rho^\dagger$ this similarity transformation is unitary, as is usual in quantum mechanics. The transformation relating the LP and field-like bases,

$$\begin{aligned} \hat{\mathbf{r}}^{(1/2)} &= \omega_k^{1/2} \hat{\mathbf{r}}^{(0)} \omega_k^{-1/2}, \\ \psi_{\mathbf{r}, \sigma}^{(1/2)}(\mathbf{k}) &= \omega_k^{1/2} \psi_{\mathbf{r}, \sigma}^{(0)}(\mathbf{k}), \\ \psi_{\mathbf{r}, \sigma}^{(-1/2)}(\mathbf{k}) &= \omega_k^{-1/2} \psi_{\mathbf{r}, \sigma}^{(0)}(\mathbf{k}), \end{aligned} \quad (18)$$

is also a similarity transformation that preserves eigenvalues. Thus the fact that the eigenvalues of the Hermitian operator $\hat{\mathbf{r}}^{(0)}$ are real thus implies that the eigenvalues of $\hat{\mathbf{r}}^{(\pm 1/2)}$ are also real. The inner-product (17) is equal to (16), so the inner-product is also preserved by the similarity transformation. The transformation (18) is not unitary and the operator $\hat{\mathbf{r}}^{(1/2)}$ is not Hermitian. This is outside the scope of the usual quantum mechanical formalism, but there has been considerable work done on pseudo-Hermitian Hamiltonians in recent years.¹³

7. POSITION EIGENVECTORS

We can define operators that annihilate or create a photon at position \mathbf{r} and time t as

$$\hat{\psi}_{\mathbf{r}, \sigma, j}^{(\alpha)}(t) \equiv \sum_{\mathbf{k}} (\omega_k)^\alpha e_{\mathbf{k}, \sigma, j}^{(\chi)} a_{\mathbf{k}, \sigma} \frac{e^{i\mathbf{k} \cdot \mathbf{r} - i\omega_k t}}{\sqrt{V}}, \quad (19)$$

$$\hat{\psi}_{\mathbf{r}, \sigma, j}^{(\alpha)\dagger}(t) \equiv \sum_{\mathbf{k}} (\omega_k)^\alpha e_{\mathbf{k}, \sigma, j}^{(\chi)*} a_{\mathbf{k}, \sigma}^\dagger \frac{e^{-i\mathbf{k} \cdot \mathbf{r} + i\omega_k t}}{\sqrt{V}}. \quad (20)$$

These are proportional to field operators if $\alpha = 1/2$ and to the vector potential operator if $\alpha = -1/2$. They satisfy the equal time commutation relations

$$\sum_j \left[\hat{\psi}_{\mathbf{r}, \sigma, j}^{(-\alpha)}(t), \hat{\psi}_{\mathbf{r}', \sigma', j}^{(\alpha)\dagger}(t) \right] = \delta_{\sigma, \sigma'} \delta^3(\mathbf{r} - \mathbf{r}'), \quad (21)$$

analogous to the displacement-potential commutation relation in QED. In terms of these operators the 1-photon localized basis states are

$$|\psi_{\mathbf{r}, \sigma}^{(\alpha)}(t)\rangle = \hat{\psi}_{\mathbf{r}, \sigma}^{(\alpha)\dagger}(t) |0\rangle. \quad (22)$$

If these position eigenvectors are projected onto the orthonormal momentum-helicity basis states $|\mathbf{k}, \sigma\rangle$, their \mathbf{k} -space representation is found to be

$$\begin{aligned} \psi_{\mathbf{r}, \sigma, j}^{(\alpha)}(\mathbf{k}, t) &= \langle \mathbf{k}, \sigma | \hat{\psi}_{\mathbf{r}, \sigma}^{(\alpha)\dagger}(t) | 0 \rangle = \langle \mathbf{k}, \sigma | \left(\sum_{\mathbf{k}'} (\omega_{k'})^\alpha e_{\mathbf{k}', \sigma, j}^{(\chi)*} \frac{e^{-i\mathbf{k}' \cdot \mathbf{r} + i\omega_{k'} t}}{\sqrt{V}} | \mathbf{k}', \sigma \rangle \right) \\ &= (\omega_k)^\alpha e_{\mathbf{k}, \sigma, j}^{(\chi)} \frac{e^{i\mathbf{k} \cdot \mathbf{r} - i\omega_k t}}{\sqrt{V}}. \end{aligned} \quad (23)$$

This is the Heisenberg picture (HP) equivalent of Eq. (11).

8. WAVE FUNCTION

A coordinate space wave function is the projection of the state vector onto a basis of position eigenvectors. A QED state vector expanded in the number-momentum-helicity basis is

$$|\Psi\rangle = c_0 |0\rangle + \sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}^\dagger |0\rangle + \frac{1}{2!} \sum_{\mathbf{k},\sigma;\mathbf{k}',\sigma'} \sqrt{\mathcal{N}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}} c_{\mathbf{k},\sigma;\mathbf{k}',\sigma'} a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k}',\sigma'}^\dagger |0\rangle + \dots \quad (24)$$

where $c_0 = \langle 0|\Psi\rangle$, $c_{\mathbf{k},\sigma} \equiv \langle 0|a_{\mathbf{k},\sigma}|\Psi\rangle$, $c_{\mathbf{k},\sigma;\mathbf{k}',\sigma'} \equiv c_{\mathbf{k}',\sigma';\mathbf{k},\sigma} = \langle 0|a_{\mathbf{k},\sigma}a_{\mathbf{k}',\sigma'}|\Psi\rangle$, and $\mathcal{N}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'} = 1 + \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$. Division by $2!$ corrects for identical states obtained when the $\{\mathbf{k},\sigma\}$ subscripts are permuted while $\sqrt{\mathcal{N}}/2$ normalizes doubly occupied states.

The 1-photon wave function is found by projecting (24) onto (22) to give

$$\begin{aligned} \Psi_\sigma^{(\alpha)}(\mathbf{r}, t) &= \langle \psi_{\mathbf{r},\sigma}^{(\alpha)} | \Psi \rangle \\ &= \sum_{\mathbf{k}} c_{\mathbf{k},\sigma} \mathbf{e}_{\mathbf{k},\sigma}^{(\chi)}(\omega_k)^\alpha \frac{e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_k t}}{\sqrt{V}}, \end{aligned} \quad (25)$$

where we are interested in the cases $\alpha = 0$ (LP) and $\alpha = \pm 1/2$ (fields and vector potential). It can be verified that these wave functions satisfy

$$i \frac{\partial \Psi_\sigma^{(-1/2)}(\mathbf{r}, t)}{\partial t} = \Psi_\sigma^{(1/2)}(\mathbf{r}, t), \quad (26)$$

which is analogous to $\mathbf{E} = -\partial\mathbf{A}/\partial t$ in the Coulomb gauge in free space. Using $i\hat{\mathbf{k}} \times \mathbf{e}_{\mathbf{k},\sigma}^{(0)} = \sigma \mathbf{e}_{\mathbf{k},\sigma}^{(0)}$ with $\mathbf{e}_{\mathbf{k},\sigma}^{(0)}$ given by (10), it follows that

$$i \frac{\partial \Psi_\sigma^{(\alpha)}(\mathbf{r}, t)}{\partial t} = \sigma c \nabla \times \Psi_\sigma^{(\alpha)}(\mathbf{r}, t) \quad (27)$$

for any α .

To obtain the 2-photon wave function we can project $|\Psi\rangle$ onto the 2-photon real space basis

$$|\psi_{\mathbf{r},\sigma,j}(t), \psi_{\mathbf{r}',\sigma',j'}(t')\rangle = \hat{\psi}_{\mathbf{r},\sigma,j}^{(\alpha)\dagger}(t) \hat{\psi}_{\mathbf{r}',\sigma',j'}^{(\alpha)\dagger}(t') |0\rangle$$

as

$$\Psi_{\sigma,\sigma';j,j'}^{(\alpha)}(\mathbf{r}, \mathbf{r}'; t, t') = \langle 0 | \hat{\psi}_{\mathbf{r},\sigma,j}^{(\alpha)}(t) \hat{\psi}_{\mathbf{r}',\sigma',j'}^{(\alpha)}(t') | \Psi \rangle. \quad (28)$$

Use of Eq. (20) and $[a_{\mathbf{k},\sigma}, a_{\mathbf{k}',\sigma'}^\dagger] = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$ to evaluate $\langle 0 | \hat{\psi}_{\mathbf{r},\sigma,j}^{(\alpha)}(t) \hat{\psi}_{\mathbf{r}',\sigma',j'}^{(\alpha)}(t') a_{\mathbf{k},\sigma''}^\dagger a_{\mathbf{k}',\sigma'''}^\dagger |0\rangle$ then gives

$$\begin{aligned} \Psi_{\sigma,\sigma';j,j'}^{(\alpha)}(\mathbf{r}, \mathbf{r}'; t, t') &= \frac{1}{2!V} \sum_{\mathbf{k},\sigma;\mathbf{k}',\sigma'} \sqrt{\mathcal{N}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}} c_{\mathbf{k},\sigma;\mathbf{k}',\sigma'} (\omega_k \omega_{k'})^\alpha \\ &\times \left(e_{\mathbf{k},\sigma,j}^{(\chi)} e_{\mathbf{k}',\sigma',j'}^{(\chi)} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_k t} e^{i\mathbf{k}'\cdot\mathbf{r}' - i\omega_{k'} t'} + e_{\mathbf{k}',\sigma',j}^{(\chi)} e_{\mathbf{k},\sigma,j'}^{(\chi)} e^{i\mathbf{k}\cdot\mathbf{r}' - i\omega_k t'} e^{i\mathbf{k}'\cdot\mathbf{r} - i\omega_{k'} t} \right) \end{aligned} \quad (29)$$

which becomes a 2-photon wave function if we set $t' = t$. A separate symmetrization step is not required since its symmetric form is a direct consequence of the commutation relations satisfied by the photon annihilation and creation operators.

A photon density operator that counts photons by first annihilating and then recreating a helicity σ photon at \mathbf{r} , time t can be defined as

$$\hat{n}_\sigma^{(\alpha)}(\mathbf{r}, t) = \hat{\psi}_{\mathbf{r},\sigma}^{(\alpha)\dagger}(t) \cdot \hat{\psi}_{\mathbf{r},\sigma}^{(-\alpha)}(t). \quad (30)$$

The expectation value of this number density operator is

$$\begin{aligned} n_\sigma^{(\alpha)}(\mathbf{r}, t) &= \langle \Psi | \hat{n}_\sigma(\mathbf{r}, t) | \Psi \rangle \\ &= \sum_j \langle \Psi | \hat{\psi}_{\mathbf{r},\sigma,j}^{(\alpha)\dagger}(t) \hat{\psi}_{\mathbf{r},\sigma,j}^{(-\alpha)}(t) | \Psi \rangle. \end{aligned} \quad (31)$$

The 0-photon contribution to n is 0, while the 1-photon contribution is

$$n_{\sigma}^{(\alpha)}(\mathbf{r}, t) = \Psi_{\sigma}^{(\alpha)*}(\mathbf{r}, t) \cdot \Psi_{\sigma}^{(-\alpha)}(\mathbf{r}, t). \quad (32)$$

For the 2-photon state (28), substitution of (21) gives

$$n_{\sigma}^{(\alpha)}(\mathbf{r}, t) = \sum_{\sigma'; j, j'} \int d^3 r' \Psi_{\sigma, \sigma'; j, j'}^{(\alpha)*}(\mathbf{r}, \mathbf{r}'; t, t) \Psi_{\sigma, \sigma'; j, j'}^{(-\alpha)}(\mathbf{r}, \mathbf{r}'; t, t),$$

implying that unobserved photons are summed over. A similar argument can be applied to each n -photon term. Photons are noninteracting particles and the existence of a photon density is consistent with Feynman's conclusion the photon probability density can be interpreted as particle density. The $\alpha = \pm 1/2$ photon density is not necessarily real or positive definite. A real density can be obtained by averaging the $\alpha = 1/2$ and $\alpha = -1/2$ densities, equivalent to taking the real part of $n_{\sigma}^{(\alpha)}(\mathbf{r}, t)$.⁴ Only the $\alpha = 0$ density is strictly positive definite, however.

For a negligibly small detector of volume ΔV , the probability that a photon is present in the detector is $n_{\sigma}^{(\alpha)}(\mathbf{r}, t) \Delta V$. To compare with Glauber photodetection theory we can consider a pulse travelling in the z -direction that is normally incident on a detector of thickness Δz and area ΔA with $\Delta V = \Delta A \Delta z$. The Glauber count rate is given by (3) and $(dn_G/dt) \Delta z/c$ is the probability the photon will be counted during the time that it takes to traverse the detector. Since $n_{\sigma}^{(1/2)} = i\epsilon_0 \mathbf{E}_{\sigma}^{(-)} \cdot \mathbf{A}_{\sigma}^{(+)}/\hbar$ where $A_{\sigma}^{(+)} \approx -iE_{\sigma}^{(+)}/\omega$ for most beams available in the laboratory, the predictions of the present photon number based theory and Glauber photodetection theory are usually indistinguishable.

9. FIELDS AND MAXWELL EQUATIONS

If we identify the operators $\hat{\Psi}^{(-1/2)}$ and $\hat{\Psi}^{(1/2)}$ with the vector potential and displacement operators as

$$\begin{aligned} \hat{\Psi}_{\sigma}^{(-1/2)}(\mathbf{r}, t) &= \sqrt{\frac{2\epsilon_0}{\hbar}} \hat{\mathbf{A}}_{\sigma}^{(+)}(\mathbf{r}, t), \\ \hat{\Psi}_{\sigma}^{(1/2)}(\mathbf{r}, t) &= -i\sqrt{\frac{2}{\hbar\epsilon_0}} \hat{\mathbf{D}}_{\sigma}^{(+)}(\mathbf{r}, t), \end{aligned} \quad (33)$$

the commutation relations (21) are in agreement with the commutation relations satisfied by $\hat{\mathbf{A}}_{\sigma}^{(+)}$ and $\hat{\mathbf{D}}_{\sigma}^{(-)}$ in QED. When one of these field operators acts on the vacuum state as in (22), the result is a 1-photon position eigenvector. The magnetic induction operator can be defined as $\mathbf{B}_{\sigma}^{(+)} = \nabla \times \mathbf{A}_{\sigma}^{(+)}$ giving

$$\begin{aligned} \mathbf{A}_{\sigma}^{(+)}(\mathbf{r}, t) &= \langle 0 | \hat{\mathbf{A}}_{\mathbf{r}, \sigma}^{(+)} | \Psi \rangle, \\ \mathbf{D}_{\sigma}^{(+)}(\mathbf{r}, t) &= \langle 0 | \hat{\mathbf{D}}_{\mathbf{r}, \sigma}^{(+)} | \Psi \rangle, \\ \mathbf{B}_{\sigma}^{(+)}(\mathbf{r}, t) &= \langle 0 | \hat{\mathbf{B}}_{\mathbf{r}, \sigma}^{(+)} | \Psi \rangle. \end{aligned} \quad (34)$$

These positive frequency wave functions satisfy MEs. For definite helicity states in free space $\mathbf{D}_{\sigma}^{(+)}/\sqrt{\epsilon_0} = i\sigma \mathbf{B}_{\sigma}^{(+)}/\sqrt{\mu_0} = \mathbf{F}_{\sigma}^{(+)}/\sqrt{2}$ where $\mathbf{F}_{\sigma}^{(+)} = \mathbf{D}_{\sigma}^{(+)}/\sqrt{2\epsilon_0} + i\sigma \mathbf{B}_{\sigma}^{(+)}/\sqrt{2\mu_0}$ is the the Reimann-Silberstein (RS) wave function.^{5, 11} Provided we work with definite helicity states, the RS and electric or magnetic field forms of the wave function are all equivalent.

In a medium the polarization and magnetization must also be considered⁴ and the vacuum state can be replaced with the zero photon state with all matter in its ground state. If the multipolar Hamiltonian is used, the vector potential operator includes a matter part, $\hat{\mathbf{A}}_m^{(+)}$, and the positive frequency vector potential can be written as $\hat{\mathbf{A}}^{(+)}(\mathbf{r}, t) = \hat{\mathbf{A}}_1^{(+)}(\mathbf{r}, t) + \hat{\mathbf{A}}_{-1}^{(+)}(\mathbf{r}, t) + \hat{\mathbf{A}}_m^{(+)}(\mathbf{r}, t)$. In a nonmagnetic medium, $\hat{\mathbf{H}} = \hat{\mathbf{B}}/\mu_0$ and

$\hat{\mathbf{D}} = \epsilon_0 \hat{\mathbf{E}} + \hat{\mathcal{P}}$ where $\hat{\mathcal{P}}^{(+)}$ annihilates a matter excitation, analogous to the annihilation of a photon. The 1-photon MEs for the positive frequency fields become

$$\begin{aligned}\nabla \cdot \mathbf{B}^{(+)} &= 0, \quad \nabla \times \mathbf{E}^{(+)} = -\frac{\partial \mathbf{B}^{(+)}}{\partial t}, \\ \nabla \cdot \mathbf{D}^{(+)} &= 0, \quad \nabla \times \mathbf{H}^{(+)} = \mathcal{P}^{(+)} + \frac{\partial \mathbf{D}^{(+)}}{\partial t}.\end{aligned}\tag{35}$$

These are equivalent to the equations obtained by Sipe⁸ using an extension of the Glauber photodetection argument.

The density $\Psi_\sigma^{(1/2)*} \cdot \Psi_\sigma^{(-1/2)} = i\epsilon_0 \mathbf{E}^{(-)} \cdot \mathbf{A}^{(+)} / \hbar$ has appeared before in the classical context and in applications to beams. Cohen-Tannoudji et. al.¹⁴ transform the classical electromagnetic angular momentum as

$$\begin{aligned}\mathbf{J} &= \epsilon_0 \int d^3 r \mathbf{r} \times (\mathbf{E} \times \mathbf{B}) \\ &= \epsilon_0 \int d^3 r \left[\sum_{i=1}^3 E_i (\mathbf{r} \times \nabla) A_i + \mathbf{E} \times \mathbf{A} \right]\end{aligned}\tag{36}$$

by requiring that the fields go to zero sufficiently quickly at infinity. Although this looks like an expectation value, the fields are classical. In a discussion of optical beams, van Enk and Nienhuis¹⁵ separate monochromatic fields into their positive and negative frequency parts using

$$\mathbf{V} = \left[\mathbf{V}^{(+)} \exp(-i\omega t) + \mathbf{V}^{(-)} \exp(i\omega t) \right] / \sqrt{2}$$

and obtain for total field linear momentum and AM

$$\mathbf{P} = -i \int d^3 r \left[\sum_{i=1}^3 D_i^{(+)*} (i\nabla) A_i^{(+)} \right],\tag{37}$$

$$\mathbf{J} = -i \int d^3 r \left[\sum_{i=1}^3 D_i^{(+)*} (-\mathbf{r} \times i\nabla + \mathbf{S}) A_i^{(+)} \right].\tag{38}$$

Here we have assumed the absence of matter in writing $\mathbf{D} = \epsilon_0 \mathbf{E}$, substituted $\mathbf{A}^{(+)} = i\omega \mathbf{D}^{(+)}$, and changed the notation a bit for consistency with the present work. These are classical expressions, but terms at frequency 2ω do not contribute to the total momentum and angular momentum, \mathbf{P} and \mathbf{J} .¹⁶ They look like the expectations values of the linear and angular momentum operators that would be obtained using the biorthonormal wave function pair $\sqrt{\epsilon_0/\hbar} \mathbf{A}^{(+)}$ and $-i\mathbf{D}^{(+)} / \sqrt{\epsilon_0 \hbar}$ in agreement with Eq. (33).

10. PHOTON WAVE MECHANICS

Photon wave mechanics follows the usual rules, as outlined by Barut and Marlin¹⁷ for example: (a) A wave equation, (27)

$$i\partial \Psi_\sigma^{(\alpha)}(\mathbf{r}, t) / \partial t = \sigma c \nabla \times \Psi_\sigma^{(\alpha)}(\mathbf{r}, t),$$

exists. The negative frequency solution can be eliminated on physical grounds, thus cutting the Hilbert space in half as is done for solutions to the Dirac equation. (b) The inner-product of the wave functions describing states $|\tilde{\Psi}\rangle$ and $|\Psi\rangle$,

$$\langle \tilde{\Psi}^{(\alpha)} | \Psi^{(-\alpha)} \rangle = \sum_\sigma \int d^3 r \tilde{\Psi}_\sigma^{(\alpha)*}(\mathbf{r}, t) \cdot \Psi_\sigma^{(-\alpha)}(\mathbf{r}, t),\tag{39}$$

exists and is invariant under similarity transformations between the $\alpha = \pm 1/2$ and the $\alpha = 0$ bases. (c) The number and current densities

$$\begin{aligned} n^{(\alpha)}(\mathbf{r}, t) &= \sum_{\sigma} \Psi_{\sigma}^{(\alpha)*} \cdot \Psi_{\sigma}^{(-\alpha)}, \\ \mathbf{j}^{(\alpha)}(\mathbf{r}, t) &= -i\sigma c \sum_{\sigma} \Psi_{\sigma}^{(\alpha)*} \times \Psi_{\sigma}^{(-\alpha)}, \end{aligned} \quad (40)$$

satisfy the continuity equation

$$\frac{\partial n^{(\alpha)}(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{j}^{(\alpha)}(\mathbf{r}, t) = 0. \quad (41)$$

This can be verified using the wave equation. The density $n^{(0)} = \sum_{\sigma} |\Psi_{\sigma}^{(0)}|^2$ is positive definite, while $[n^{(1/2)}, \mathbf{j}^{(1/2)}]$ is a 4-vector that can be written as the contraction of second rank EM field tensors with 4-potentials. (d) The momentum operator is $\hbar \mathbf{k}$ and the position operator is given by Eq. (13) in \mathbf{k} -space. (e) The eigenvectors of the position operator are δ -function normalized. (f) The position operator and inner-product give the density $\langle \psi_{\mathbf{r}, \sigma}^{(\alpha)} | \Psi \rangle^* \langle \psi_{\mathbf{r}, \sigma}^{(-\alpha)} | \Psi \rangle$.

11. ANGULAR MOMENTUM AND BEAMS

The physical interpretation of the position eigenvectors³ was motivated by the recent experimental and theoretical work on optical vortices,¹² and AM is central to an understanding of position eigenvectors. The expansion of the unit vectors $\mathbf{e}_{\mathbf{k}, \sigma}^{(\chi)}$ in Eq. (15) shows that the unit vectors contribute AM $\{s_z, l_z\}$ equal to $\{-1, m\sigma + 1\}$, $\{0, m\sigma\}$ or $\{1, m\sigma - 1\}$ with probability amplitudes $(\cos \theta - \sigma)/2$, $\sin \theta/\sqrt{2}$ and $(\cos \theta + \sigma)/2$ respectively to a definite helicity localized state. For every term the z -component of total AM is $\hbar j_z$ with $j_z = m\sigma$, that is total AM has a definite value, but spin and orbital AM do not. The position eigenvectors must have orbital AM, and this implies a vortex structure that can be moved from positive to the negative z -axis depending on the choice of χ , but not eliminated.

Theoretically, the simplest beams with orbital AM are the nondiffracting Bessel beams (BBs), and these beams are closely related to our localized states. BBs satisfy MEs and have definite frequency, ck_0 , and a definite wave vector, k_z , along the propagation direction. It then follows that the \mathbf{k} -space transverse wave vector magnitude $k_{\perp} = \sqrt{k_0^2 - k_z^2}$, and the angle $\theta = \tan^{-1}(k_{\perp}/k_z)$ also have definite values. Cylindrical symmetry is retained when integrating over ϕ by weighting all ϕ equally with phase factor $\exp(im\phi)$. When Fourier transformed to \mathbf{r} -space the modes go as $\exp(-ik_0 ct + il_z \varphi + ik_z z) J_{l_z}(k_{\perp} r)$ where $l_z = m$ and $m \pm 1$ in (15), J_{l_z} are Bessel functions, φ the real space azimuthal angle, and r is the perpendicular distance from the beam axis.¹⁸ If integrated over k_{\perp} the result is a sum of outgoing and incoming waves that is localized on the z -axis at some instant in time. If the BBs are then integrated over k_z , the result is equivalent to a sum over all positive and negative wave vectors, and states localized in three dimensions are obtained. If we select $\chi = 0$ so that the \mathbf{k} -space unit vectors are $\hat{\phi}$ and $\hat{\theta}$ in the linear polarization basis, \mathbf{B} is transverse to $\hat{\mathbf{z}}$ for the $\hat{\theta}$ mode and \mathbf{E} is transverse for the $\hat{\phi}$ mode and the linearly polarized modes can be called transverse magnetic (TM) and transverse electric (TE) respectively.

A paraxial beam propagating in the $\hat{\mathbf{z}}$ -direction with frequency ω , helicity σ , and z -component of orbital AM $\hbar l_z$ can be described in cylindrical polar coordinates by the vector potential¹⁹

$$\mathbf{A}^{(+)}(\mathbf{r}, t) = \frac{1}{2} (\hat{\mathbf{x}} + i\sigma \hat{\mathbf{y}}) u(r) \exp[i l_z \varphi + i k_z (z - ct)]. \quad (42)$$

This vector potential is equivalent to the wave function $\Psi_{\sigma'}(\mathbf{r}, t) = \delta_{\sigma, \sigma'} \sqrt{2\epsilon_0/\hbar} \mathbf{A}^{(+)}(\mathbf{r}, t)$. The z -component of the time average of the classical AM density, equal to $\mathbf{r} \times (\mathbf{D}^{(-)} \times \mathbf{B}^{(+)})$, is then found to be

$$J_z(r) = \epsilon_0 \left[\omega l_z |u(r)|^2 - \frac{1}{2} \omega \sigma r \frac{\partial |u(r)|^2}{\partial r} \right]. \quad (43)$$

This can be interpreted as the quantum mechanical AM density in a 1-photon state. The first term of (43) is consistent with orbital AM $\hbar l_z$ per photon since the photon density given by (32) reduces to $n^{(1/2)}(\mathbf{r}, t) = \epsilon_0 \omega |u(r)|^2 / \hbar$. The last term of (43) does not look like photon spin density. The most paradoxical case is a plane wave. For example a wave function proportional to $(\hat{\mathbf{x}} + i\sigma\hat{\mathbf{y}}) \exp(ikz - i\omega t)$ implies linear momentum $\hbar k\hat{\mathbf{z}}$ per photon and hence no z -component of AM. The AM of this beam resides in its edges, as can be seen from Eq. (43) and a new edge is created if the disk intercepts part of the beam, reducing the AM of the beam.²⁰ Based on the derivation here, this result applies not only to a classical beam, but also to a 1-photon state.

12. SUMMARY

We have derived 1 and 2-photon wave functions from QED by projecting the state vector onto the eigenvectors of a photon position operator. Largely because it is still widely believed that there is no position operator, this is the first time that photon wave functions have been obtained in this way. While only the LP wave function gives a positive definite photon density, field-like wave functions are widely used and are more convenient in many applications. In the field-like definite helicity basis the wave function pair is given by (33), with $\Psi_\sigma^{(\alpha)}$ are given by (25). The linear polarization basis of TM and TE fields can be obtained by taking the sum and difference of the definite helicity modes as in (23). The 1-photon density is $n_\sigma^{(\alpha)}(\mathbf{r}, t) = \Psi_\sigma^{(\alpha)*} \cdot \Psi_\sigma^{(-\alpha)}$, where $n_\sigma^{(1/2)}$ is essentially equal to $n_\sigma^{(0)}$ except for very broad band signals. This can be generalized to describe the photon density in a multiphoton state using the expectation value of the number operator, (31).

Systematic investigation of photon position operators and their eigenvectors clarifies the role of the photon wave function in classical and quantum optics. The LP wave function is related to field based wave functions through a similarity transformation that preserves eigenvalues and scalar products. The field $\mathbf{D}^{(+)}(\mathbf{r}, t)$ is proportional to the Glauber wave function which gives the photodetection amplitude for a detector that responds to the electric field. Fields and potentials are locally related to charge and current sources, and hence are the most convenient in many applications. However, Fourier transformation of \mathbf{k} -space probability amplitudes naturally leads to the LP form.²¹ Selection of the LP or field-potential is a matter of convenience in most applications.

By the general rules of quantum mechanics the LP wave function gives the probability to detect a photon at a point in space. It and the closely related field-potential wave function pair obtained by solution of MEs are ideally suited to the interpretation of photon counting experiments using a detector that is small in comparison with the spatial variations of photon density. It is not subject to limitations based on nonlocalizability, and coarse graining or restriction to length scales smaller than a wave length is not required. Exact localization in vacuum requires infinite energy and is not physically possible, but position eigenvectors provide a useful mathematical description of photon density. Photon number density is equivalent to integration over undetected photons in a multiphoton beam. Our formalism justifies the use of positive frequency solutions to MEs as photon wave functions and gives a rigorous theoretical basis for extrapolation of their range of applicability from the many photon to the 1-photon regime.

ACKNOWLEDGMENTS

The author acknowledges the financial support of the Natural Science and Engineering Research Council of Canada.

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